Understanding the complex patterns of snow crystals

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Abstract

We will show that the complex shapes of snow crystals can be explained from a simple basic mechanism that is also responsible for the appearance of many others structures in nature. We expect that this new physical mechanism, that follows from minimizing the total stored energy, will permit to explain most of the features of snow crystal growth.

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Up to now, we all have admired snowflakes and other beautiful examples of solidification patterns, but the physical mechanism responsible for this structures has remained a mystery. In this work we will unveil the underlying basic mechanism responsible for the spontaneous pattern formation in the growth of crystals. We will provide an example of evolution of a macroscopic pattern obtained using a numerical implementation of the basic equations, starting from a single point and evolving in a deterministic way towards a complex branched structure.

Real snow crystals often come with a six-fold symmetrical shape as a consequence that the most typical basic form of an ice crystal is an hexagonal prism. Other basic forms occur at very low temperatures or very high pressures.

A typical planar dendritic ice crystal showing the six-fold symmetry is shown in Fig. 1. Snow crystals grow from condensing water vapor in the air, around a nucleus of dust. In their travel from cloud towards ground, these crystals pass through various temperature regimes. If ambient temperature is cold enough, their arms grow very rapidly, and if temperature warms up, the arms are capped, spreading outward slightly, until the next cold temperature regime causes them to grow again. What we see landing at earth surface are snowflakes, formed by snow cristals aglomerations produced at warmer zones of the atmosphere.

The observation of snowflakes and these sub-millimeter snow crystals can be traced to 1611 with the work of Johannes Kepler entitled "The Six-Cornered Snowflake" [1]. After that, several authors have continued the work of observing, cataloging, taking photos, and growing artificial snow crystals in the laboratory [2, 3, 4, 5, 6, 7, 8, 9, 10]. The preliminary observations together with the latest systematic observations and experiments, have provided the basis for understanding the basic mechanism responsible for the creation of these fascinating structures.

For the theoretical description of crystal growth, and reviews on the vast subject of pattern formation, we will refer the reader toward Refs. [11, 12, 13, 14, 15]. For alternative models of crystal growth we refer the reader toward Refs. [16, 17, 18].

The key point for understanding the physics governing crystal growth comes from studying from an unified point of view, several apparently different physical systems. We studied several pattern forming systems in which the normal growth velocity is proportional to the gradient of a bulk field which obeys a Laplace or diffusion type of equation. Some examples are: dielectric breakdown, streamers, solidification, crystal growth, viscous fingers, biolog-

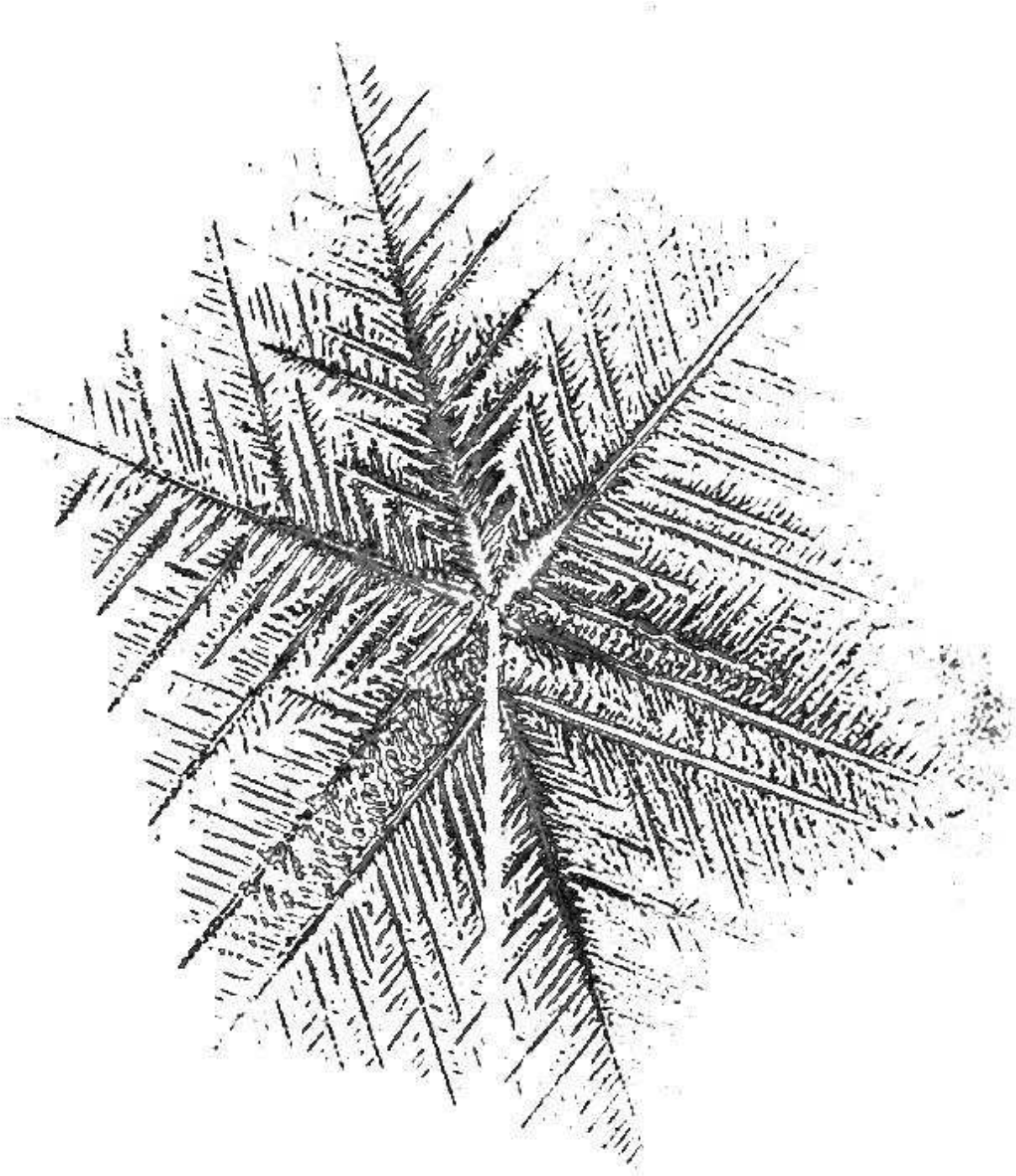

Figure 1: Photograph of dendritic ice crystal grown in pure water at an undercooling of TM - T = 2.34°C (Original by T. Fujioka, reproduced from Langer 1980. We altered the background of this image).

ical patterns, combustion, etc. The origin of structures in these systems is known to be related to the Mullins-Sekerka instability [19, 20]. This instability explain why a protrusion in the interface causes the interface to grow faster there, but the theory for the evolution of a growing protrusion towards complex structures has remained a mystery. In this work we will show that the underlying basic mechanism responsible for spontaneous pattern formation, needs to consider the global evolution of the system and not just to study the evolution of a local protrusion. It is not true that just a protrusion grows faster, and depending on some physical parameters, sometimes is energetically favorable for the system to develop other branches after some size of the protrusion is reached.

In the theoretical study of the evolution of an interface, the simplest possibility is to expand the growing interface towards regions of maximum temperature gradient. This necessarily gives a straight line as a consequence of the Mullins-Sekerka instability mentioned previously. We will show that it is possible to obtain a branched structure starting from a central seed, following a quasi-stationary deterministic treatment, that only relies in minimizing the total energy stored in the system, and changing locally the thermal conductivity of the medium at each step of iteration.

The energy stored in the temperature field can be obtained from

$$U = \frac{1}{2} \int k(\nabla T \cdot \nabla T) dV. \tag{1}$$

By analogy with dielectric breakdown [21], we can study systems with boundary conditions for the temperature T at the inner and outer interface, by letting them to evolve towards regions of higher U. This turn out to be equivalent to the evolution towards a pattern that minimize the total stored energy, after a local change in the thermal conductivity k.

The energy U can be obtained as follows: First, impose the boundary conditions: T= 0 in the inner seed and T= 1 in the outer interface. Second, impose a fixed constant value for the thermal conductivity in all the region between the outer interface and the seed. Third, solve the Laplace equation

$$\nabla \cdot (k \nabla T) = 0, \tag{2}$$

obtaining the temperature T in the region between the outer interface and the seed. Fourth, obtain the gradients of T, and using Eq. 1, obtain the energy U.

Now we will study the evolution of a central seed in the circular geometry of Fig. 2. We

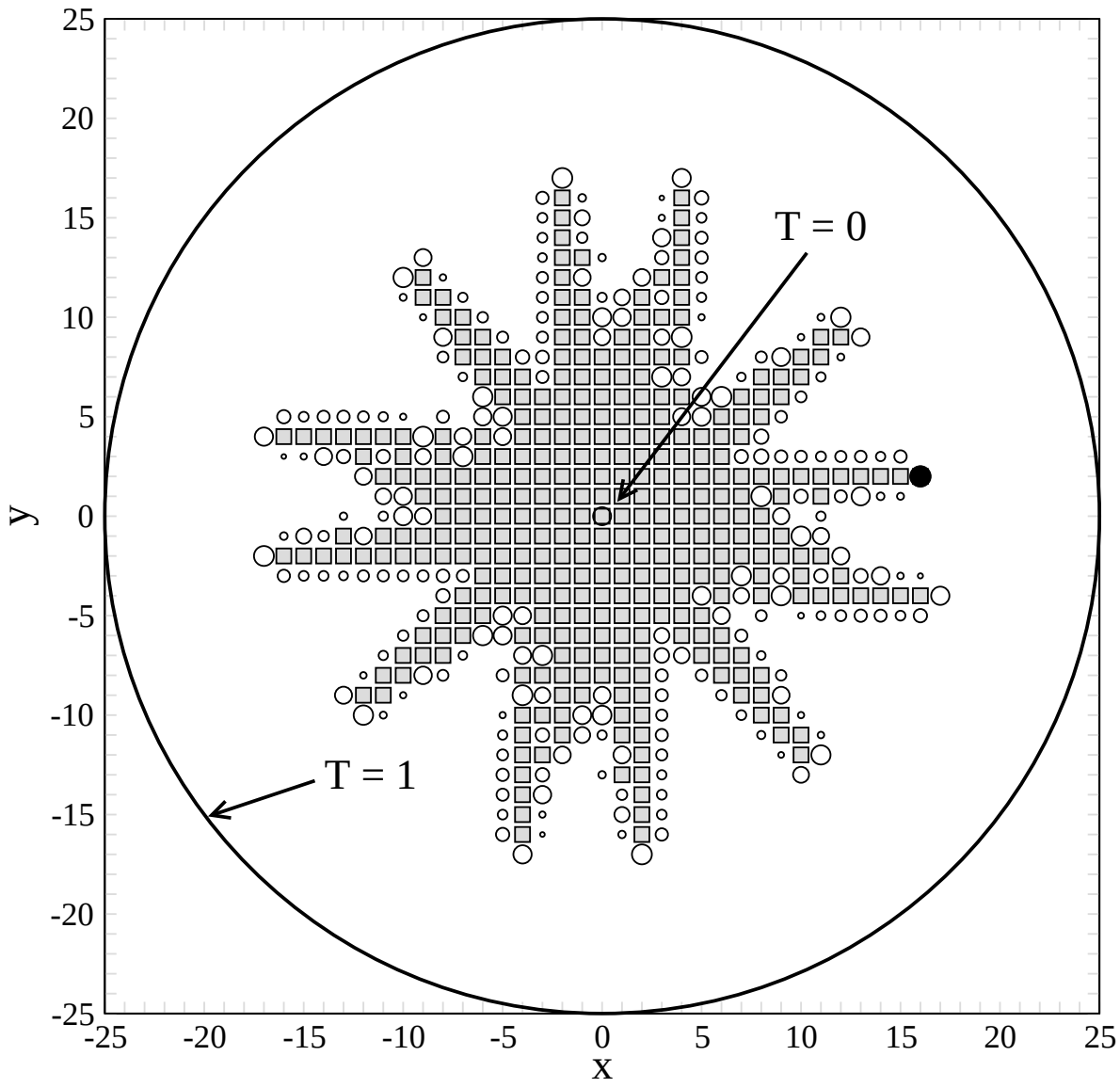

Figure 2: Schematic view of the two-dimensional circular geometry used in our calculations. The central circle represents the seed and the big circle the outer interface. Filled boxes represent the evolving pattern (sites where the thermal conductivity is greater). The circles show all possible sites where the pattern can evolve, the diameter of each of these circles represent the value for the energy U of the system in case this site is added to the pattern. The black circle at the right of the figure is the next step in the evolution of this pattern.

consider a two-dimensional square lattice, where the central point is the seed and the outer interface is modeled as a discretized version of the big circle. The boundary conditions, T=0 in the seed and T=1 in the outer interface, are maintained trough all the steps in our simulation. The first step is to assign a fixed value for the thermal conductivity of each lattice point between the seed and the outer interface, and set the initial pattern as the central point. The second step is to obtain the energies U of the system after changing the thermal conductivity in one of each neighbor of the pattern to a greater value k', these energies are compared and the neighbor providing the bigger energy value is added to the pattern. To maintain the model simple, pattern evolution through the diagonals are not permitted. The pattern grows adding a site to the evolving pattern each time the last step is repeated. The filled boxes represent the evolving pattern (sites where the thermal conductivity is k'). The circles show all possible sites where the pattern can evolve, the diameter of each of these circles represent the value for the energy U of the system in case this site is added to the pattern. The black circle at the right of the figure shows the site giving the biggest contribution to U, and is the next step in the evolution of this pattern. System parameters are the same as those used for obtaining Fig. 3, see below.

Fig. 3 shows the structure of the pattern for a 70x70 square lattice after 750 iterations. For each different configuration, the numerical solution of Eq. 2 was accepted when the numerical residual was less than 10^{-1}, the values for the thermal conductivity outside the channel was k =2 and inside the channel was k'=6. The evolution of the pattern shows that opposite branches are not exactly aligned, we consider this as a prediction of our model and with a little bit of imagination it is possible to find this effect in the experimental results shown in Fig. 1. Our example also shows that the system develops, forming initially a central structured core, this core supports the evolution of the main venous branches and diagonal branches. We expect that secondary branches emerging from the main branches will appear after some iterations, resembling the branches shown in Fig. 1. Our simulated structure doesn't show the six-fold symmetry of real snow crystals, this is a consequence of using a square lattice in our numerical model. We expect that realistic six-fold patterns will be formed in a lattice that impose the hexagonal symmetry. We have not tested our model changing the supporting lattice, because several months of computing time was needed for completing this example. Repetitive calculations, or calculations using bigger lattices, would require to implement sophisticated numerical methods [22].

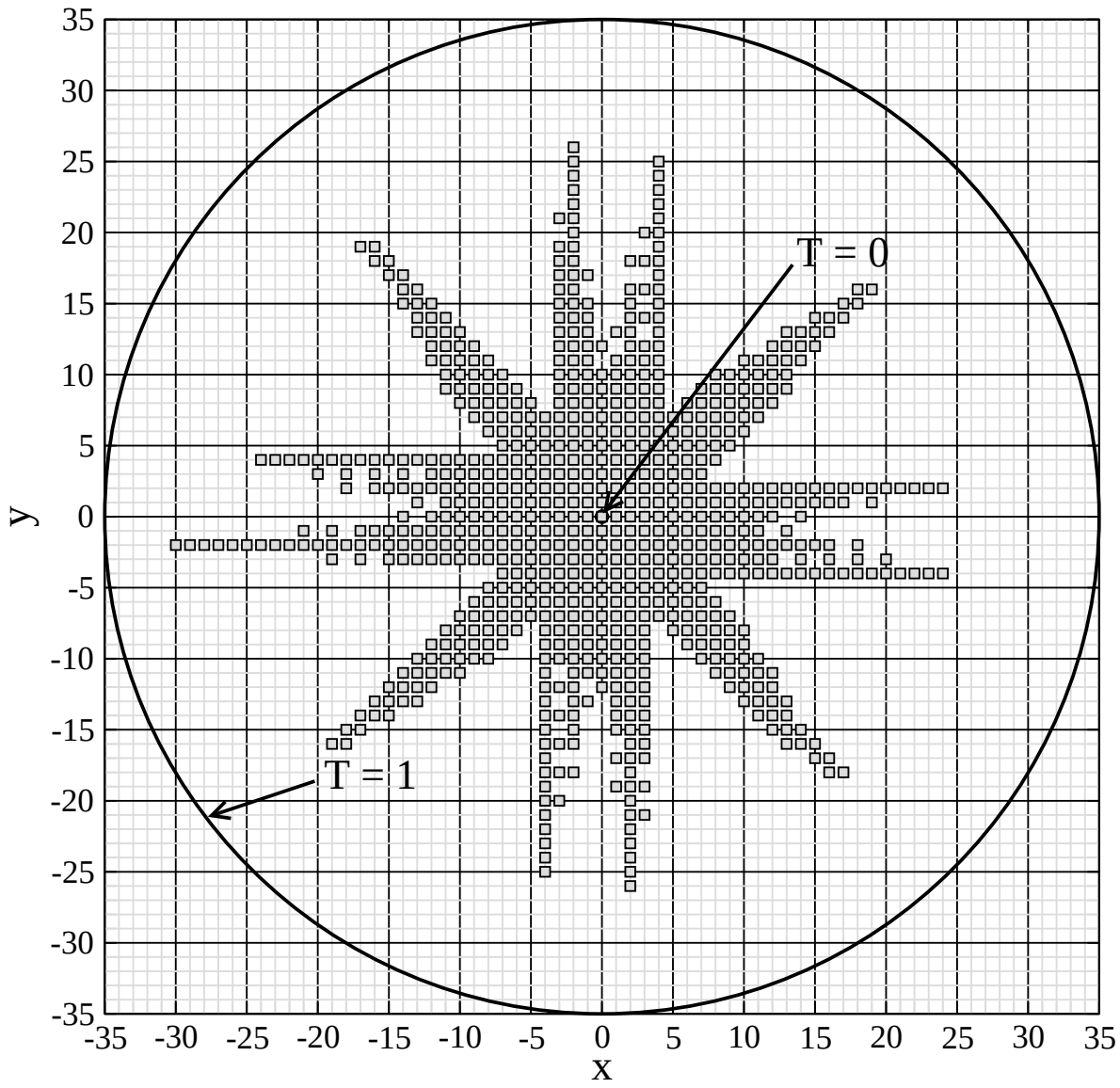

Figure 3: Pattern developed for a 70 x 70 square lattice after 750 iterations for thermal conductivity outside the channel k =2 and inside the channel k'=6.

The large computing time needed for these simulations is a consequence of the necessity for the system to probe different possible configurations and select the one minimizing the total stored energy. This is the famous principle of minima action that is nicely explained in the textbook of Richard Feynman [23]. In normal systems, like a mass falling towards the earth surface as a consequence of the force of gravity, this principle leads to simple differential equations for the motion of particles. In the case studied in this article there

are not trajectories emerging from this principle, instead there are complex configurations of the inner interface as a result of minimizing the total stored energy. We expect that, at least for some specific examples, our discretized model could evolve towards a continuum theory in the future. In either case the fundamental principles discussed in this paper would help to explain many systems developing complex structures.

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